Influence of fluorine substituents on the electronic properties of selenium-N-heterocyclic carbene compounds

ABSTRACT

N-heterocyclic carbenes (NHCs) are common ancillary ligands in organometallic compounds that are used to alter the electronic and steric properties of a metal centre. To date, various NHCs have been synthesised with different electronic properties, which can be done by modifying the backbone or changing the nitrogen substituents group. This study describes a systematic modification of NHCs by the inclusion of fluorine substituents and examines the use of selenium-NHC compounds to measure the π-accepting ability of these fluorinated NHC ligands. Evaluation of the 77Se NMR chemical shifts of the selenium adducts reveals that fluorinated NHCs have higher chemical shifts than the non-fluorinated counterparts, IMes and IPh. Higher 77Se NMR chemical shifts values indicate a stronger π-accepting ability of the NHC ligands. The findings of this study suggest that the presence of fluorine atoms has increased the π-accepting ability of the corresponding NHC ligands. This work supports the advantage of the 77Se NMR chemical shifts of selenium-NHC compounds for assessing the influence of fluorine substituents on NHC ligands.

Keyword: N-heterocyclic carbene; Selenium; Fluorine; NMR spectroscopy